HYDRAULIC CONDUCTIVITY ESTIMATION IN PARTIALLY SATURATED SOILS USING THE ADJOINT METHOD

J. SANTOS*, Y. EFENDIEV†, AND L. GUARRACINO‡

Abstract An iterative algorithm based on the adjoint method for the estimation of the saturated hydraulic conductivity k in a partially saturated soil Q is proposed. Groundwater flow in Q is assumed to be described by Richards equation. The optimization problem minimizes the L^2-error between the pressure head values $p(k, x, t)$ calculated as the solution of a direct problem and the measured values of the pressure head at discrete points inside the domain Q. The exact gradient of the cost functional is obtained by solving an appropriate adjoint problem, which is derived from the equations of the Gâteaux derivatives of the pressure head with respect to the parameter k. A finite element procedure is used to obtain approximate solutions of the direct and adjoint problems and the Gâteaux derivatives. A discrete form of expression of the gradient of the cost functional at the continuous level is used inside a nonlinear conjugate gradient iteration to solve the optimization problem. A numerical example showing the implementation of the algorithm to estimate the saturated hydraulic conductivity $k(x)$ during an hypothetical infiltration experiment in a heterogeneous soil is also presented.

KEYWORDS: Inverse Problems, Adjoint Methods, Finite Elements.

1. Introduction. In recent years, understanding and quantifying the global hydrologic cycle has become a priority research. Soil moisture, in particular, has gained a lot of attention as it constitutes a key variable in the global hydrologic cycle. Soil moisture is most often described as the moisture in the top several meters of soil that can interact with the atmosphere through evapotransportation, infiltration, and runoff. Soil moisture conditions are important in determining the amount of infiltration, runoff, and groundwater recharge. In addition, land-atmosphere processes critically depend on the state of soil moisture, as soil moisture partitions the energy of fluxes available at the land surfaces into latent and sensible heat fluxes.

Accurate assessment of the spatial and temporal variation of soil moisture are advantageous for numerous applications and for answering diverse research questions. Measurement of soil moisture is important for the study and understanding of all surface biogeophysical processes. This includes agriculture, environment, ecology, water resources, climate dynamics, soil strength and soil erosion. For example, in climate dynamics, long-term changes in soil moisture stores have been identified as an indicator of climate change, and soil moisture information can calibrate and validate global climate models. Given the critical role that soil moisture plays in most land-surface processes, it is desirable that soil moisture be monitored with the same accuracy and frequency as other important environmental variables.

*Department of Mathematics, Purdue University, West Lafayette, IN 47907-1395 and Facultad de Ciencias Astronomicas y Geofisicas, Universidad Nacional de La Plata, Paseo del Bosque, S/N, (1900) La Plata, Argentina,

†Department of Mathematics, Texas A & M University, College Station, TX 77843-3368,

‡Facultad de Ciencias Astronomicas y Geofisicas, Universidad Nacional de La Plata, Paseo del Bosque, S/N, (1900) La Plata, Argentina

Numerical modeling of soil moisture requires an accurate knowledge of the hydraulic conductivity and water content functions. These characteristic functions are usually described by empirical mathematical models with different number of fitting parameters, such as Brooks-Corey [1] or van Genuchten [2] models. Model parameters are often difficult or even impossible to measure directly because of instrumentation, scale or conceptual constraints. Thus, inverse modeling of laboratory or field data has become an attractive alternative to direct measurements [3, 4, 5, 6]. In recent years, various optimization methods such quasi-Newton [7], Simplex [4], Levenberg-Marquardt [6, 8] and Ant Colony [9] have been used for parameter estimation of characteristic curves. In particular, the estimation of the saturated hydraulic conductivity is rather critical because the groundwater flow is highly sensitive to this parameter [10]. Hydraulic conductivity values are relatively easy to obtain from laboratory methods but these values are often non-representative of *in-situ* conditions [11].

Traditionally, *in-situ* moisture measurement techniques provide point measurements. Though these measurements do not account for the spatial variability of the typical soil moisture profiles. Because *in-situ* soil moisture measurements are generally expensive and often problematic, no large-scale soil moisture networks exist to measure soil moisture at the ideal high frequency, multiple depths, and fine spatial resolution that is needed for complete understanding of soil moisture dynamics.

The objective of this paper is to present a nonlinear optimization algorithm to determine the saturated hydraulic conductivity field (the parameter to be estimated), based on local measurements. Groundwater flow is assumed to be described by Richards equation [12] in conjunction with the van Genuchten model. The optimization problem minimizes the L^2-error between the pressure head values $p(x, k, t)$ calculated at the measurements points and the measured values of the pressure head at these discrete points. The gradient of the cost functional in our nonlinear optimization problem is defined at the continuous level using the adjoint of the Gâteaux derivative of the solution with respect to the parameter. Both the Gâteaux derivative and the adjoint are defined at the continuous level as solutions of partial differential equations with appropriate initial and boundary conditions and then discretized using finite element procedures. This approach, known as *differentiate-then-discretize*, provides an expression for the gradient which is independent of the particular discretization algorithm used to solve the differential problems. This method has been used for example, in [13, 14, 15, 16, 17, 18] to solve parameter estimation problems in geophysics and other applications. For an account of several aspects of parameter estimation such as regularization, identifiability, etc, we refer to [19]. In particular, the proposed adjoint procedure allows for a more accurate calculation of the gradient of the cost functional than the standard *discretize-then-differentiate* approach consisting in discretizing the differential equations first and then applying optimization techniques to a discrete version as described for example in [20].

The organization of the paper is as follows. Section 2 states Richards equation in terms of the pressure head $p(k)$ as a function of saturated hydraulic conductivity $k(x)$ that will be the parameter to be estimated. The analysis of the inverse problem and results on the continuity and differentiability of $p(k)$ with respect to the parameter $k(x)$ are presented in Section 3. Section 4 is devoted to the formulation of the adjoint problem and the derivation of an expression of the gradient of the cost functional that will be used in the discrete minimization procedure. In Section 5, a Newton iteration to solve the continuous minimization problem is formulated and analyzed.

The formulation of the discrete parameter estimation algorithm employing a nonlinear conjugate gradient algorithm is done in Section 6. Section 7 presents numerical experiments showing the application of the proposed algorithm to estimate the saturated hydraulic conductivity in a vertical soil profile. Finally, the Appendix contains the proof of the continuity of the parameter to output mapping $k \to p(k)$.

2. The direct model and the parameter estimation problem. We consider the problem of estimating the saturated hydraulic conductivity $k(x)$ in a multidimensional bounded variably saturated soil Q with boundary ∂Q. Let Γ^* be the part of ∂Q associated with the top surface of the soil, i.e., the part of ∂Q, where the rain and evapotranspiration data will be specified and we set $\Gamma = \partial Q \setminus \Gamma^*$.

It will be assumed that water flow within Q is governed by Richards equation [12] stated in the form

$$D_t\theta(p(k)) - div(kg(p(k))D_x(p(k) + x_3)) = 0, \quad x \in Q, \quad t \in I = (0,T), \tag{2.1}$$

with boundary conditions

$$\begin{aligned} -kg(p(k))D_x(p(k) + x_3) \cdot \nu &= q^*, \quad x \in \Gamma^*, \quad t \in I, \\ -kg(p(k))D_x(p(k) + x_3) \cdot \nu &= 0, \quad x \in \Gamma, \quad t \in I, \end{aligned} \tag{2.2}$$

and initial conditions

$$p(k)(t = 0) = p_0(x),\ x \in Q. \tag{2.3}$$

In the equations above ν denotes the unit outward normal to ∂Q , $g(p)$ is the relative hydraulic conductivity and the x_3-axis is considered to be positive upward. In the rest of the paper, it will be assumed that there exists positive constants c_1, c_2, c_3, c_4 such that

$$0 < c_1 < kg(p(k)) < c_2, \tag{2.4}$$

$$0 < c_3 < (D_p\theta)(p(k)) < c_4. \tag{2.5}$$

To solve the differential problem (2.1)–(2.3), the functions $\theta(p)$ and $g(p)$ need to be specified. One of the commonly used pairs $(\theta(p), g(p))$ is given by the van Genucthen model [2]:

$$\theta(p) = \begin{cases} \dfrac{\theta_s - \theta_r}{[1 + (\alpha_{vg}|p|)^n]^m} + \theta_r, & \text{for} \quad p < 0 \\ \theta_s & \text{for} \quad p \geq 0, \end{cases} \tag{2.6}$$

$$g(p) = \begin{cases} \dfrac{\{1 - (\alpha_{vg}|p|)^{n-1}[1 + (\alpha_{vg}|p|)^n]^{-m}\}^2}{[1 + (\alpha_{vg}|p|)^n]^{m/2}} & \text{for} \quad p < 0 \\ 1 & \text{for} \quad p \geq 0, \end{cases} \tag{2.7}$$

where θ_r and θ_s are the residual and saturated water contents, respectively; n and α_{vg} are shape parameters; and m is given by the relation $m = 1 - 1/n$.

Next, we formulate our parameter estimation problem. Assume that the pressure head values $(p(x_{ri}, t))_{1 \leq i \leq N_r}$ are recorded at the points x_{ri} inside Q for all $t \in I$.

Then our objective is to use the observation vector $p^{obs}(t) = ((p(x_{ri},t))_{1\le i\le N_r}$ to infer the actual values of the saturated hydraulic conductivity $k(x)$. We will consider the set of admissible parameters to be

$$\mathcal{P} = \{k : k \text{ is measurable},\ \ k_* \le k(x) \le k^*\}$$

endowed with the $L^2(Q)$-topology, where K_* and K^* are positive constants.

We consider the cost functional $\mathcal{J}(k)$ defined as follows. For each point x_{ri} let B_i be a small ball of radius ρ small enough such that $B_i \cap B_j = \emptyset$, $i \ne j$. Then let us define

$$\begin{aligned} \widehat{p}(k, x_{ri}, t) &= \frac{1}{|B_i|}\int_{B_i} p(k,x,t)dx, \\ \widehat{p}(k,t) &= (p(k,x_{ri},t))_{1\le i\le N_r} \in R^{N_r}. \end{aligned} \tag{2.8}$$

Then let $\mathcal{J}(k)$ be defined by

$$\mathcal{J}(k) = \frac{1}{2}\|\widehat{p}(k) - p^{obs}\|_{L^2(I,R^{N_r})}. \tag{2.9}$$

Our estimation problem solved using a least squares criterion will be

$$\text{minimize} \quad \mathcal{J}(k) \quad \text{over} \quad \mathcal{P}. \tag{2.10}$$

3. Analysis of the minimization problem. Let us consider the parameter-to-output mapping that associates to each element k the corresponding solution $p(k,x,t)$ of (2.1)–(2.3).

Consider (2.1) for two different hydraulic conductivities k_1 and k_2:

$$\begin{aligned} D_t\theta(p(k_1)) - div(k_1 g(p(k_1))D_x(p(k_1)+x_3)) = 0, \\ D_t\theta(p(k_2)) - div(k_2 g(p(k_2))D_x(p(k_2)+x_3)) = 0, \end{aligned} \tag{3.1}$$

and subtract them:

$$\begin{aligned} D_t(\theta(p(k_1)) - \theta(p(k_2))) - div(k_1 g(p(k_1))D_x(p(k_1)+x_3)) \\ + div(k_2 g(p(k_2))D_x(p(k_2)+x_3)) = 0. \end{aligned} \tag{3.2}$$

For simplicity of notations, we denote $p_1 = p(k_1)$ and $p_2 = p(k_2)$, and for any function $f(p(k))$, $f(p_1) = f(p(k_1)), f(p_2) = f(p(k_2))$. After adding and subtracting the term $div(k_2 g(p_2)D_x(p_1+x_3))$ in (3.2), defining

$$\zeta(k_1,k_2) = k_1\left[g(p_1) - g(p_2)\right] + g(p_2)\left[k_1 - k_2\right], \tag{3.3}$$

and denoting

$$d_p(k_1,k_2) = p_1 - p_2,$$

equation (3.2) can be rewritten as

$$\begin{aligned} D_t\left[\theta(p_1) - \theta(p_2)\right] - div(k_2 g(p_2) D_x d_p(k_1,k_2)) \\ = div(\zeta(k_1,k_2)D_x(p_1+x_3)), \quad x \in Q, \quad t \in I, \end{aligned} \tag{3.4}$$

or in the equivalent form

$$
\begin{aligned}
&(D_p\theta)(p_2)D_t d_p(k_1,k_2) + \left[(D_p\theta)(p_1) - (D_p\theta)(p_2)\right] D_t p_1 \\
&\quad -div(k_2 g(p_2) D_x d_p(k_1,k_2)) \\
&\quad = div(\zeta(k_1,k_2) D_x(p_1 + x_3)), \quad x \in Q, \quad t \in I,
\end{aligned} \tag{3.5}
$$

with the following boundary and initial conditions

$$
-k_2 g(p_2) D_x d_p(k_1,k_2)\cdot\nu = \zeta(k_1,k_2) D_x(p_1 + x_3)\cdot\nu,\ x \in \Gamma^*,\ t \in I, \tag{3.6}
$$

$$
-k_2 g(p_2) D_x d_p(k_1,k_2)\cdot\nu = 0, \quad x \in \Gamma,\ t \in I, \tag{3.7}
$$

$$
d_p(k_1,k_2)(t=0) = 0, \quad x \in Q. \tag{3.8}
$$

For simplicity of the notations in further analysis, we use the notation

$$
d_f(k_1,k_2) = f(p(k_1)) - f(p(k_2)). \tag{3.9}
$$

The following theorem shows the continuity of the parameter-to-output mapping when the set of admissible parameters $\mathcal{P}$ is endowed with the $L^2(Q)$-topology.

Theorem 3.1. *Assume that there exists a positive constant c_5 such that $\|D_t^{(n)} p(k)\|_{L^\infty(I,L^\infty(Q))} \le c_5$, $n = 0,1,2,3$ and $\|D_x D_t^{(n)} p\|_{L^\infty(I,L^\infty(Q))} \le c_5$, $n = 0,1,2$. Also assume that $(D_p^{(n)}\theta)(p)$, $n = 1,2,3$ and $(D_p^{(n)} g)(p)$, $n = 0,1,2$ are bounded and Lipschitz continuous functions of p. Then the solution $d_p(k_1,k_2)$ of (3.5) with the boundary and initial conditions (3.6)-(3.8) exists and is unique and satisfies the estimates*

$$
\begin{aligned}
&\|D_t^{(n)} d_p(k_1,k_2)\|_{L^\infty(I,L^2(Q))} + \|D_x D_t^{(n)} d_p(k_1,k_2)\|_{L^2(I,L^2(Q))} \\
&\quad \le c\|k_1 - k_2\|_{L^2(Q)}, \quad n = 0,1,2.
\end{aligned} \tag{3.10}
$$

The proof of this theorem is presented in Appendix A. Note that the assumption imposed on p requires higher regularity of k. Consequently, the admissible set $\mathcal{P}$ is a subset of $L^2(Q)$. The higher regularity conditions are required for the proof of Theorem 3.4.

As a consequence of Theorem 3.1, we obtain the following result.

Lemma 3.1. *Under the assumptions of Theorem 3.1, the mapping*

$$
\begin{aligned}
(\mathcal{P}, L^2(Q)) &\to L^\infty(I, H^n(Q)) \bigcap L^2(I, H^{n+1}(Q)) \\
k &\to p(k)
\end{aligned} \tag{3.11}
$$

is continuous for $n = 0,1,2$, where $H^0 = L^2$.

The validity of following theorem concerning the existence of solutions of our least squares problem (2.10) is an immediate consequence of Lemma 3.1.

Theorem 3.2. *Let $A \subset \mathcal{P}$ be a compact set on $L^2(Q)$. Then the problem*

$$
\min_A \mathcal{J}(k)
$$

has a solution.

To solve the parameter estimation problem later we will define an iterative procedure requiring the calculation of the Gâteaux derivative $D_k(p)\delta k$ of the pressure head $p(k,x,t)$ with respect to the parameter k.

It will be assumed that the parameter $k(x)$ is known in a small neighborhood B_0 of Γ^*. Thus, the space of perturbations δk of the parameter k will be chosen to be the space

$$\delta\mathcal{P}_0 = \{\delta k \in L^2(Q) \quad \text{such that} \quad \delta k(x) = 0 \text{ for } x \in B_0\}, \tag{3.12}$$

endowed with the $L^2(Q)$-topology.

We will show in Theorem 3.4 below that

$$p(k + \lambda\delta k) = p(k) + D_k(p)\lambda\delta k + \phi(k, k + \lambda\delta k), \tag{3.13}$$

where $D_k(p)$ is the linear operator defined from $\delta\mathcal{P}_0$ into $L^\infty(I, L^2(Q)) \bigcap L^2(I, H^1(Q))$ and

$$\frac{\|\phi(k, k + \delta k)\|_{L^\infty(I,L^2(Q)) \bigcap L^2(I,H^1(Q))}}{\lambda} \to 0 \tag{3.14}$$

as λ tends to zero.

To demonstrate the validity of (3.13)-(3.14), for any $\delta k \in \mathcal{P}_0$, we first define $\Phi = \Phi(k) = D_k(p)\delta k$, as the solution of the equation

$$\begin{aligned} D_t(D_p(\theta)\Phi) - div(kg(p(k))D_x\Phi) - div((kD_p(g)\Phi)D_x(p + x_3)) = \\ div(g(p(k))\delta k D_x(p(k) + x_3)), \quad x \in Q,\ t \in I, \end{aligned} \tag{3.15}$$

with the boundary condition

$$-kg(p(k))D_x\Phi \cdot \nu = 0, \quad x \in \partial Q,\ t \in I, \tag{3.16}$$

and the initial condition

$$\Phi(\cdot, t = 0) = 0, \quad x \in Q. \tag{3.17}$$

Since $\delta k \in \delta\mathcal{P}_0$, a weak formulation for (3.15)- (3.17) is as follows: find $\Phi \in H^1(Q)$ such that

$$\begin{aligned} &(D_t(D_p(\theta)\Phi), v) + (kg(p(k))D_x\Phi, D_x v) + ((kD_p(g)\Phi)D_x(p(k) + x_3), D_x v) \\ &\quad = -(g(p(k))\delta k D_x(p(k) + x_3), D_x v), \quad \forall v \in H^1(Q). \end{aligned} \tag{3.18}$$

Theorem 3.3. *Under the assumptions of Theorem 3.1, for any $\delta k \in \delta\mathcal{P}_0$ there exists a unique solution $\Phi = D_k(p)\delta k$ of (3.15)-(3.17) and satisfies the following estimate*

$$\|D_t^{(n)}\Phi\|_{L^\infty(I,L^2(Q))} + \|D_x D_t^{(n)}\Phi\|_{L^2(I,L^2(Q))} \le c\|\delta k\|_{L^2(Q)},\ n = 0, 1, 2, \tag{3.19}$$

so that in particular $D_k(p)\delta k \in L^2(I, L^2(Q))$ and

$$D_k(p) : \delta\mathcal{P}_0 \to L^2(I, L^2(Q))$$

is a continuous linear operator.

The proof of this theorem is similar to the proof of Theorem 3.1. In particular, following the proof of Theorem 3.1, one can show that (3.19) holds for $\delta k \in L^\infty(Q) \cap \delta\mathcal{P}_0$. Further, applying the Hahn-Banach theorem, this result can be extended to $\delta k \in \delta\mathcal{P}_0$.

To show the validity of (3.13)-(3.14), we will demonstrate that

$$\phi = \phi(k + \lambda\delta k, k) = \Phi - \frac{d_p(k + \lambda\delta k, k)}{\lambda}$$

converges to zero as $\lambda \to 0$ in $L^\infty(I, L^2(Q)) \bigcap L^2(I, H^1(Q))$. Taking $k_1 = k + \lambda\delta k$, $k_2 = k$ in (3.4), with $\delta k \in \delta\mathcal{P}_0$, dividing by λ and subtracting the resulting equation from (3.15), we obtain that ϕ satisfies the following differential equation.

$$\begin{aligned} D_t\left(D_p(\theta)\Phi - \frac{d_\theta(k + \lambda\delta k, k)}{\lambda}\right) - div(kg(p(k))D_x\phi) \qquad (3.20) \\ = div\left((kD_p(g)\Phi + g(p(k))\delta k)D_x(p(k) + x_3)\right) \\ -div\left([(k + \lambda\delta k)\frac{d_g(k + \lambda\delta k, k)}{\lambda} + g(p(k))\delta k]D_x(p(k + \lambda\delta k) + x_3)\right), \; x \in Q, \, t \in I. \end{aligned}$$

Also, subtracting (3.6) for the same choice of k_1 and k_2 from (3.16), we get the following boundary conditions for ϕ:

$$-kg(p(k))D_x\phi \cdot \nu = 0, \quad x \in \partial Q, \; t \in I. \qquad (3.21)$$

Moreover, we have the following initial condition (cf. (3.8))

$$\phi(\cdot, t = 0) = 0, \quad x \in Q. \qquad (3.22)$$

THEOREM 3.4. *Assume the conditions of Theorem 3.1 are satisfied. Then, the solution ϕ of (3.20)–(3.22) satisfies*

$$\|\phi\|_{L^\infty(I,L^2(Q))} + \|D_x\phi\|_{L^2(I,L^2(Q))} \to 0 \qquad (3.23)$$

as $\lambda \to 0$, provided $\delta k \in L^\infty(Q) \bigcap \delta\mathcal{P}_0$.

Proof.

For further calculations, we denote

$$\begin{aligned} R_1 = -[kD_p(g)\Phi + g(p(k))\delta k]D_x(p(k) + x_3) + \\ [(k + \lambda\delta k)\frac{d_g(k + \lambda\delta k, k)}{\lambda} + g(p(k))\delta k]D_x(p(k + \lambda\delta k) + x_3). \end{aligned} \qquad (3.24)$$

It can be shown that the equation (3.20) has the following variational form

$$\begin{aligned} \left(D_t\left(D_p(\theta)\Phi - \frac{d_\theta(k + \lambda\delta k, k)}{\lambda}\right), \psi\right) + (kg(p(k))D_x\phi, D_x\psi) \qquad (3.25) \\ = (R_1, D_x\psi), \quad \psi \in H^1(Q). \end{aligned}$$

The fact that there are no boundary terms from the integration by parts of the last term can be verified directly. In the proof we will use the following identity which holds for any smooth function $\Psi(p) \in C^2(R)$,

$$\begin{aligned} \Psi(p(k + \lambda\delta k)) = \Psi(p(k)) + D_p(\Psi)(p(k))(p(k + \lambda\delta k) - p(k)) + \\ D_p^{(2)}(\Psi)(p^*_\lambda)(p(k + \lambda\delta k) - p(k))^2, \end{aligned} \qquad (3.26)$$

where $p^*_\lambda = p(k+\lambda_0\delta k)$ for some λ_0 between 0 and λ. This identity can be also written as

$$d_\Psi(k+\lambda\delta k,k) = D_p(\Psi)(p(k))(p(k+\lambda\delta k)-p(k)) \\ +D_p^{(2)}(\Psi)(p^*_\lambda)(p(k+\lambda\delta k)-p(k))^2. \tag{3.27}$$

Applying (3.27) to d_θ in (3.25), we have

$$(D_t\left[D_p(\theta)\phi\right],\psi) - (D_t\left(\frac{D_p^{(2)}(\theta)(p^*_\lambda)d_p(k+\lambda\delta k,k)^2}{\lambda}\right),\psi) \\ +(kg(p(k))D_x\phi, D_x\psi) = (R_1, D_x\psi). \tag{3.28}$$

Taking $\psi=\phi$ in (3.28) we have

$$(D_t(D_p(\theta)\phi),\phi) - (D_t\left(\frac{D_p^{(2)}(\theta)(p^*_\lambda)d_p(k+\lambda\delta k,k)^2}{\lambda}\right),\phi) \\ +(kg(p(k))D_x\phi, D_x\phi) = (R_1, D_x\phi).$$

The equation above can be written as

$$\frac{1}{2}D_t((D_p(\theta)\phi,\phi)) + \frac{1}{2}(\phi^2, D_t(D_p(\theta))) - (D_t\left(\frac{D_p^{(2)}(\theta)(p^*_\lambda)d_p(k+\lambda\delta k,k)^2}{\lambda}\right),\phi) \\ +(kg(p(k))D_x\phi, D_x\phi) = (R_1, D_x\phi). \tag{3.29}$$

From (3.29) we have

$$D_t\|D_p(\theta)^{1/2}\phi\|^2_{L^2(Q)} + \|D_x\phi\|^2_{L^2(Q)} \\ \le c\bigg(\|\phi\|^2_{L^2(Q)} + \|R_1\|^2_{L^2(Q)} + \frac{1}{\lambda^2}\|d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)} \\ +\frac{1}{\lambda^2}\|D_t d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)}\bigg). \tag{3.30}$$

To estimate $\|R_1\|^2_{L^2(Q)}$ on the right-hand side of (3.30), we write R_1 as

$$R_1 = g(p(k))\delta k D_x d_p(k+\lambda\delta k,k) \\ +k\left(\frac{d_g(k+\lambda\delta k,k)}{\lambda} - D_p(g)D_k(p)\delta k\right)D_x(p(k+\lambda k)+x_3) \\ +\delta k\ d_g(k+\lambda\delta k,k)D_x(p(k+\lambda k)+x_3) + k\ D_p(g)\Phi D_x d_p(k+\lambda\delta k,k). \tag{3.31}$$

Using (3.27)

$$d_g(k+\lambda\delta k,k) = D_p(g)(p(k))d_p(k+\lambda\delta k,k) \\ +D_p^{(2)}(g)(p^{**}_\lambda)d_p(k+\lambda\delta k,k)^2, \tag{3.32}$$

where $p^{**}_\lambda = p(k+\lambda_0\delta k)$ for some λ_0 between 0 and λ, we have the following estimate for the second term on the right hand side of (3.31)

$$
\begin{aligned}
&\|D_p(g)D_k(p)\delta k - \frac{d_g(k+\lambda\delta k,k)}{\lambda}\|_{L^2(Q)} \\
&\quad \le c\Big(\|D_p(g)[D_k(p)\delta k - \frac{d_p(k+\lambda\delta k,k)}{\lambda}]\|_{L^2(Q)} + \|D_p^{(2)}(g)(p_\lambda^{**})\frac{d_p(k+\lambda\delta k,k)^2}{\lambda}\|_{L^2(Q)}\Big) \\
&\quad = c\Big(\|D_p(g)\phi\|_{L^2(Q)} + \|D_p^{(2)}(g)(p_\lambda^{**})\frac{d_p(k+\lambda\delta k,k)^2}{\lambda}\|_{L^2(Q)}\Big) \\
&\quad \le c\|\phi\|_{L^2(Q)} + \frac{c_1}{\lambda}\|d_p(k+\lambda\delta k,k)\|^2_{L^4(Q)},
\end{aligned}
$$

since $D_x p(k), D_p(g)$ and $D_p^{(2)}(g)$ are bounded functions.

Next, the using that $g(p)$ and δk are in $L^\infty(Q)$, the L_2-norm of first term on the right hand side of (3.31) can be bounded by

$$
c\|D_x d_p(k+\lambda\delta k,k)\|_{L^2(Q)}.
$$

Also, since $g(p)$ is a Lipschitz continuous function and $\|D_x p\|_{L^\infty(Q)}$ is bounded, the L^2-norm of the third term on the right hand side of (3.31) can be bounded by

$$
c(\|d_p(k+\lambda\delta k,k)\|^2_{L^4(Q)} + \|d_p(k+\lambda\delta k,k)\|_{L^2(Q)}).
$$

To bound the last term on the right hand side of (3.31), first note that from Theorem 3.3 and standard elliptic regularity estimates, it follows that $\Phi \in L^\infty(I, H^2(Q))$. Because of the continuous embedding of H^2 into L^∞, we obtain $\Phi \in L^\infty(I, L^\infty(Q))$. Thus, the last term on the right hand side of (3.31) is bounded by

$$
c\|D_x d_p(k+\lambda\delta k,k)\|_{L^2(Q)}.
$$

Combining all these estimates for R_1 we have

$$
\begin{aligned}
\|R_1\|_{L^2(Q)} \le c\Big(&\|d_p(k+\lambda\delta k,k)\|_{H^1(Q)} + \|\phi\|_{L^2(Q)} + \\
&\frac{1}{\lambda}\|d_p(k+\lambda\delta k,k)\|^2_{L^4(Q)}\Big)
\end{aligned}
\tag{3.33}
$$

Thus, the estimate (3.30) becomes

$$
\begin{aligned}
&D_t\|D_p(\theta)^{1/2}\phi\|^2_{L^2(Q)} + \|D_x\phi\|^2_{L^2(Q)} \\
&\quad \le c\Big(\|\phi\|^2_{L^2(Q)} + \|d_p(k+\lambda\delta k,k)\|^2_{H^1(Q)} + \frac{1}{\lambda^2}\|d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)} \\
&\quad + \frac{1}{\lambda^2}\|D_t d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)}\Big).
\end{aligned}
\tag{3.34}
$$

Finally, using the assumption $D_p(\theta) > c_3$ and applying Gronwall's inequality we get

$$
\begin{aligned}
\max_t \|\phi\|^2_{L^2(Q)} + \|D_x\phi\|^2_{L^2(I,Q)} \le c\int_0^T \Big(&\|d_p(k+\lambda\delta k,k)\|^2_{H^1(Q)} \\
+ \frac{1}{\lambda^2}\|d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)} + \frac{1}{\lambda^2}\|D_t d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)}\Big) d\tau.
\end{aligned}
\tag{3.35}
$$

Using Theorem 3.1 we can bound the first term on the right hand side of (3.35) by $c\lambda^2$. Next, we show that the second term on the right hand side of (3.35) goes to zero as $\lambda \to 0$. For this purpose, we only need to show that

$$\int_0^T \|d_p(k+\lambda\delta k, k)/\lambda\|_{L^4(Q)} d\tau \le c_6, \tag{3.36}$$

where c_6 is independent of λ. From Theorem 3.1, we have $d_p(k+\lambda\delta k,k)/\lambda \in L^2(I, H^1(Q))$ and $D_t d_p(k+\lambda\delta k,k)/\lambda \in L^2(I,H^1(Q))$. Consequently, $d_p(k+\lambda\delta k,k)/\lambda \in C(I,H^1(Q))$ (after possibly being redefined on a set of measure zero). Because of the continuous embedding $H^1(Q) \subset L^4(Q)$ for $n = 2,3$, we obtain $d_p(k+\lambda\delta k,k)/\lambda \in L^4(I, L^4(Q))$, and

$$\int_0^T \frac{1}{\lambda^2}\|d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)} d\tau \le c\lambda^2,$$

so that (3.36) holds.

Similarly, one can show that the third term on the right hand side of (3.35) approaches to zero as $\lambda \to 0$. It follows from Theorem 3.1 that $D_t d_p(k+\lambda\delta k,k)/\lambda \in L^2(I,H^1(Q))$ and $D_t(D_t d_p(k+\lambda\delta k,k))/\lambda \in L^2(I,H^1(Q))$. Consequently, $D_t d_p(k+\lambda\delta k,k)/\lambda$ is a bounded function of the time variable and $D_t d_p(k+\lambda\delta k,k)/\lambda \in C(I,H^1(Q))$ (after possibly being redefined on a set of measure zero). Thus, $D_t d_p(k+\lambda\delta k,k)/\lambda \in L^4(I,L^4(Q))$, and we have

$$\int_0^T \frac{1}{\lambda^2}\|D_t d_p(k+\lambda\delta k,k)\|^4_{L^4(Q)} d\tau \le c\lambda^2.$$

Hence

$$\max_t \|\phi\|^2_{L^2(Q)} + \|D_x\phi\|^2_{L^2(I,Q)} \le c\lambda^2 \tag{3.37}$$

which shows the validity of (3.23). This completes the proof. □

The following theorem about the continuity of $\Phi(k) = D_k(p)\delta k$ with respect to k will be needed for the convergence analysis of the iterative estimation algorithms which are defined later. The technique of the proof of this theorem is the same as that in Theorem 3.4 and it will be omitted.

THEOREM 3.5. *Under the assumptions of Theorem 3.1, for any $\delta k \in \delta\mathcal{P}_0$ $\Phi(k) = D_k(p)\delta k$ is Lipschitz continuous with respect to k in the following sense:*

$$\|\Phi(k_1)-\Phi(k_2)\|_{L^\infty(I,L^2(Q))} + \|D_x(\Phi(k_1)-\Phi(k_2))\|_{L^2(I,L^2(Q))} \le c\|k_1-k_2\|_{L^2(Q)}. \tag{3.38}$$

4. Analysis of the adjoint problem. For the algorithm description we need the adjoint of the differential problem (3.15)-(3.17) for the Gâteaux derivative $D_k(p)\delta k$. The assumption that $\delta k \in \mathcal{P}_0$ implies that to solve the adjoint problem (3.15)-(3.17), we need to find the solution $W(k)$ of the (adjoint) differential equation

$$\begin{aligned} &-D_p(\theta)D_tW(k) - div(kg(p(k))D_xW(k)) \\ &\quad + kD_p(g)D_x(p(k)+x_3)\cdot D_xW(k) = f, \quad x\in Q,\ t\in I, \end{aligned} \tag{4.1}$$

with boundary conditions

$$kg(p(k))D_xW(k)\cdot\nu = 0 \quad x \in \partial Q,\ t\in I, \tag{4.2}$$

and final condition

$$W(k)(\cdot,T)=0, \quad x\in Q. \tag{4.3}$$

A weak form for (4.1)-(4.3) is as follows: find $W(k)\in H^1(Q)$ such that

$$\begin{aligned}&-(D_p(\theta)D_tW(k),v)+(kg(p(k))D_xW(k),D_xv) \qquad (4.4)\\&\quad+(kD_p(g)D_x(p(k)+x_3)\cdot D_xW(k),v)=(f,v), \quad v\in H^1(Q).\end{aligned}$$

The continuity of $W(k)$ with respect to the parameter k can be obtained with an argument similar to that given in Theorem 3.1.

LEMMA 4.1. *Under the hypothesis of Theorem 3.1, the solution $W(k)$ of* (4.1)-(4.3) *is Lipschitz-continuous in the following sense:*

$$\begin{aligned}&\|D_t^{(n)}d_W(k_1,k_2)\|_{L^\infty(I,L^2(Q))}+\|D_xD_t^{(n)}d_W(k_1,k_2)\|_{L^2(I,L^2(Q))}\\&\quad\le c\|k_1-k_2\|_{L^2(Q)}, \quad n=0,1,2. \qquad (4.5)\end{aligned}$$

In the next two lemmas, we derive an expression for the gradient of our cost functional $\mathcal{J}(k)$, which is needed for the definition of the discrete iterative estimation algorithm.

LEMMA 4.2. *The value of the adjoint map*

$$D_k^*(p): L^2(I,L^2(Q))\to\delta\mathcal{P}_0$$

can be computed by the relation

$$D_k^*(p)(f)=-\int_0^T g(p(k))D_x(p(k)+x_3)\cdot D_xW(k)dt, \quad f\in L^2(I,L^2(Q)), \tag{4.6}$$

where $W(k)$ is the solution of (4.1)-(4.3).

Proof.

Take $v=\Phi=D_k(p)\delta k$ with $\delta k\in\mathcal{P}_0$ as a test function in (4.4) and integrate the obtained equation from 0 to T:

$$\begin{aligned}&-\int_0^T(D_p(\theta)D_tW(k),\Phi)dt+\int_0^T\Big[(kgD_xW(k),D_x\Phi) \qquad (4.7)\\&\quad+(kD_p(g)D_x(p+x_3)\cdot D_xW(k),\Phi)\Big]dt=\int_0^T(f,\Phi)dt.\end{aligned}$$

Using integration by parts in time in the first term on the left-hand side of (4.7) and the final and initial conditions for $W(k)$ and Φ the above equation can be written as

$$\begin{aligned}&\int_0^T(W(k),D_t(D_p(\theta)\Phi))dt+\int_0^T\Big[(kgD_xW(k),D_x\Phi)+(kD_p(g)D_x(p+x_3)\cdot D_xW(k),\Phi)\Big]dt\\&\quad=\int_0^T(f,D_k(p)\delta k)dt=(\delta k,D_k^*(p)(f)). \qquad (4.8)\end{aligned}$$

Next, choosing $W(k)$ as a test function in the weak form (3.18) for Φ and integrating the resulting equation from 0 to T we obtain

$$\begin{aligned}&\int_0^T(D_t(D_p(\theta)\Phi),W(k))dt+\int_0^T(kgD_x\Phi,D_xW(k))dt \qquad (4.9)\\&\quad+\int_0^T(kD_p(g)\Phi D_x(p+x_3),D_xW(k))dt=-\int_0^T(g\delta kD_x(p+x_3),D_xW(k))dt.\end{aligned}$$

Writing the third term on the left hand side of (4.9) as

$$\int_0^T (\Phi, kD_p(g)D_x(p+x_3)\cdot D_xW(k))dt$$

from (4.8)-(4.9) we obtain

$$\begin{aligned}(\delta k, D_k^*(p)(f)) &= -\int_0^T (g\delta k D_x(p(k)+x_3), D_xW(k))dt \\ &= -(\delta k, \int_0^T g(p(k))D_x(p(k)+x_3)\cdot D_xW(k)dt), \quad \forall \delta k \in \mathcal{P}_0.\end{aligned}$$

From here, (4.6) follows.
□

LEMMA 4.3. *The functional $\mathcal{J}(k)$ has a gradient with respect to the parameter k, denoted $\mathcal{J}_k'(k) = D_k\mathcal{J}(k) : \delta\mathcal{P}_0 \to R$ which can be computed from the identity*

$$\mathcal{J}_k'(k) = D_k^*(p)f, \tag{4.10}$$

where f(x,t) is the residual-related function given by

$$f(x,t) = \sum_{i=1}^{N_r} \frac{1}{|B_i|}\chi_{B_i}(x)\left(\widehat{p}(k, x_{ri}, t) - p^{obs}(x_{ri}, t)\right). \tag{4.11}$$

In (4.11), *$\chi_{B_i}(x)$ denotes the characteristic function of the ball B_i.*

Proof.

Let $\delta k \in \delta\mathcal{P}_0$. First note that

$$\begin{aligned}\mathcal{J}(k+\delta k) &= \mathcal{J}(k) + D_k\mathcal{J}(k)\delta k + R(k+\delta k, k) \\ &= \mathcal{J}(k) + (D_k\mathcal{J}(k), \delta k)_{L^2(Q)} + R(k+\delta k, k),\end{aligned} \tag{4.12}$$

with

$$\frac{|R(k+\delta k, k)|}{\|\delta k\|_{L^2(Q)}} \to 0 \qquad \text{as} \qquad \|\delta k\|_{L^2(Q)} \to 0. \tag{4.13}$$

Since

$$\mathcal{J}(k) = \frac{1}{2}(\widehat{p}(k) - p^{obs}, \widehat{p}(k) - p^{obs})_{L^2(I, R^{N_r})},$$

using (3.13) we see that

$$\begin{aligned}\mathcal{J}(k+\delta k) = \frac{1}{2}(&\widehat{p}(k) + \widehat{D}_k(p)\delta k + \widehat{\phi}(k+\delta k, k) - p^{obs}, \\ &\widehat{p}(k) + \widehat{D}_p(k)\delta k + \widehat{\phi}(k+\delta k, k) - p^{obs})_{L^2(I, R^{N_r})} \\ = \mathcal{J}(k) &+ \int_0^T \left(\widehat{p}(k) - p^{obs}, \widehat{D}_k(p)\delta k\right)_{R^{N_r}} dt + \frac{1}{2}\|\widehat{D}_k(p)\delta k\|^2_{L^2(I, R^{N_r})} \\ &+ \left(\widehat{\phi}(k+\delta k, k), \widehat{p}(k) + \widehat{D}_k(p)\delta k + \widehat{\phi}(k+\delta k, k) - p^{obs}\right)_{L^2(I, R^{N_r})} \\ \equiv \mathcal{J}(k) &+ \int_0^T \left(\widehat{p}(k) - p^{obs}, \widehat{D}_k(p)\delta k\right)_{R^{N_r}} dt + S(k+\delta k, k),\end{aligned} \tag{4.14}$$

where

$$S(k+\delta k,k)=\frac{1}{2}\|\widehat{D}_k(p)\delta k\|^2_{L^2(I,R^{N_r})}$$
$$+\left(\widehat{\phi}(k+\delta k,k),\widehat{p}(k)+\widehat{D}_k(p)\delta k+\widehat{\phi}(k+\delta k,k)-p^{obs}\right)_{L^2(I,R^{N_r})}.$$

Next, note that using Theorem 3.3,

$$\begin{aligned}\|\widehat{D}_k(p)\delta k\|^2_{L^2(I,R^{N_r})}&=\int_0^T\sum_{i=1}^{N_r}\left|\frac{1}{|B_i|}\int_{B_i}D_k(p)\delta k(x,t)dx\right|^2dt \\ &\le c\|D_k(p)\delta k\|^2_{L^2(I,L^2(Q))}\le c\|\delta k\|^2_{L^2(Q)}.\end{aligned} \tag{4.15}$$

Next, a similar argument employing Theorem 3.4 shows that

$$\begin{aligned}&\left(\widehat{\phi}(k+\delta k,k),\widehat{p}(k)+\widehat{D}_k(p)\delta k+\widehat{\phi}(k+\delta k,k)-p^{obs}\right)_{L^2(I,R^{N_r})} \\ &\qquad\le c\|\delta k\|^2_{L^2(Q)}.\end{aligned} \tag{4.16}$$

Thus using (4.15)-(4.16) in (4.14) we conclude that

$$\frac{|S(k+\delta k,k)|}{\|\delta k\|_{L^2(Q)}}\to 0 \qquad \text{as} \qquad \|\delta k\|_{L^2(Q)}\to 0. \tag{4.17}$$

Then from (4.12)-(4.13) and (4.14)-(4.17) we see that

$$(D_k\mathcal{J}(k),\delta k)_{L^2(Q)}=\int_0^T\left(\widehat{p}(k)-p^{obs},\widehat{D}_k(p)\delta k\right)_{R^{N_r}}dt, \quad \forall\,\delta k\in\delta\mathcal{P}_0. \tag{4.18}$$

Next, note that

$$\begin{aligned}&\int_0^T\left(\widehat{p}(k)-p^{obs},\widehat{D}_k(p)\delta k\right)_{R^{N_r}}dt \\ &=\int_0^T\sum_{i=1}^{N_r}\left(\frac{1}{|B_i|}\int_{B_i}D_k(p)\delta k(x,t)\chi_{B_i}(x)dx\right)\left(\widehat{p}(k,x_{ri},t)-p^{obs}(x_{ri},t)\right)dt \\ &=\int_0^T\int_Q D_k(p)\delta k(x,t)f(x,t)dxdt \\ &=(f,D_k(p)\delta k)_{L^2(I,L^2(Q))}=(D_k^*(p)f,\delta k)_{L^2(Q)}, \quad \forall\delta k\in\delta\mathcal{P}_0.\end{aligned} \tag{4.19}$$

Now the conclusion follows from (4.18)-(4.19). ☐

Now we have the following Corollary.

Corollary 4.4. *Under the assumptions of Theorem 3.1, the continuous linear functional $\mathcal{J}_k'(k)$ is given by the equation*

$$\mathcal{J}_k'(k)(x)=-\int_0^T g(p(k))(x)D_x(p(k,x)+x_3)\cdot D_xW(k,x)dt, \quad x\in Q, \tag{4.20}$$

where $W(k)$ is the solution of (4.1)-(4.3) with f defined by (4.11)*. Also, $\mathcal{J}_k'(k)$ is Lipschitz continuous with respect to the parameter k in the following sense:*

$$\|\mathcal{J}_k'(k_1) - \mathcal{J}_k'(k_2)\|_{L^2(Q)} + \|D_x\left(\mathcal{J}_k'(k_1) - \mathcal{J}_k'(k_2)\right)\|_{L^2(Q)} \le c\|k_1 - k_2\|_{L^2(Q)}. \tag{4.21}$$

Proof. Equation (4.20) follows from Lemmas 4.2 and 4.3. Further using the fact that $g(p)$ is bounded and continuously differentiable as a function of p, and that $p(k)$ and $W(k)$ are bounded and Lipschitz continuous thanks to Theorem 3.1 and Lemma 4.1, we conclude the validity of (4.21). This completes the proof.
□

5. A Newton iteration at the continuous level. Let $\mathcal{L}(\delta\mathcal{P}_0, \delta\mathcal{P}_0)$ denote the continuous linear functionals from $\delta\mathcal{P}_0$ into itself. Following [16], for $k \in \mathcal{P}$ we define $\mathcal{M}(k) \in \mathcal{L}(\delta\mathcal{P}_0, \delta\mathcal{P}_0)$ by the rule

$$\mathcal{M}(k)\gamma = D_k^*(p)D_k(p)\gamma, \quad \gamma \in \delta\mathcal{P}_0. \tag{5.1}$$

Next, for $k \in \mathcal{P}$ such that $\mathcal{M}(k)$ has an inverse, define

$$\Lambda(k) = \left[\mathcal{M}(k)\right]^{-1} D_k^*(p)\left(p(k) - p^{obs}\right). \tag{5.2}$$

Then we define the Newton iteration by

$$k_{j+1} = \begin{cases} k_j + \Lambda(k_j), & k_* \le k_j + \Lambda(k_j) \le k^*, \\ k_*, & k_j + \Lambda(k_j) < k_*, \\ k^*, & k_j + \Lambda(k_j) > k^*. \end{cases} \tag{5.3}$$

Next, we analyze the convergence of the Newton iteration (5.3). First recall that according to Lemma 3.1 and Theorem 3.3 the mapping $k \to p(k)$ is continuous and $D_k(p) : \delta\mathcal{P}_0 \to L^2(I, L^2(Q))$ is a bounded linear operator. Also, from Theorem 3.5 we know that for $\delta k \in \delta\mathcal{P}_0$, $D_k(p)\delta k$ is a Lipschitz continuous function of k. Then, the validity of the following theorem can be established with the argument given in Theorem 4.1 of [16].

Theorem 5.1. *Assume the conditions of Theorem 3.1 are satisfied. Also assume that there exists a $k^c \in \mathcal{P}$ such that $D_k(J)(k^c) = 0$ and that $\mathcal{M}(k^c)$ is invertible. Then k^c is a point of attraction of the iteration* (5.3).

Any discrete implementation of the Newton iteration (5.3) is computationally expensive, involving the solution of as many forward problems as parameters chosen to represent the function $k(x)$. See for example [21], [22], [23] and [24]. Thus in order to solve our parameter estimation problem in the next sections, we will define a fast conjugate gradient-type iteration using a discrete version of the expression for the gradient $\mathcal{J}_k'(k)$ obtained in Lemma 4.2.

6. A discrete parameter estimation algorithm. In order to define a discrete estimation algorithm, as a first step we need to obtain approximations to the solution $p(k, x, t)$ of (2.1)–(2.3), to the Gâteaux derivative $D_k(p)\delta k(k, x, t)$ defined in (3.15)–(3.17) and to the solution $W(k, x, t)$ of the adjoint problem (4.1)–(4.3). This is done using finite element procedures as indicated below.

Let $\mathcal{M}^h$ be a finite element subspace of $H^1(Q)$ associated with a quasi-uniform partition $\mathcal{T}^h$ of Q into elements Q_j of diameter bounded by h.

Let L be a positive integer and $\Delta t = T/L$. Also, set

$$u^{h,n} = u^h(n\Delta t), \quad d_t u^{h,n} = \frac{u^{h,n+1} - u^{h,n}}{\Delta t}, \quad u^{h,n+\frac{1}{2}} = \frac{u^{h,n+1} + u^{h,n}}{2},$$

and for any function $u(p^h)$ of p^h set $u^{h,n} = u(p^h(n\Delta t))$.

The discrete-time Galerkin procedure to obtain approximations to the solution of (2.1)–(2.3) is defined using a backward Euler algorithm combined with a modified Picard iteration in time of iteration index i as indicated in what follows. Let $p(k)^{h,n+1,0} \in \mathcal{M}^h$ be an initial guess for the Picard iteration to obtain $p(k)^{h,n+1} \equiv p(k)^{h,n+1,\infty}$, which denotes the value of $p(k)^{h,n+1,i+1} \in \mathcal{M}^h$ after convergence with a prescribed tolerance in the iteration has been achieved. Then, we find $p(k)^{h,n+1,i+1} \in \mathcal{M}^h$ such that

$$\begin{aligned}
&\left(\frac{[D_p(\theta)]^{h,n+1,i}}{\Delta t} p(k)^{h,n+1,i+1}, \varphi\right) + \left(kg^{h,n+1,i} D_x p(k)^{h,n+1,i+1}, D_x\varphi\right) \qquad (6.1)\\
&= \quad -\left\langle q^{*,n+1}, \varphi\right\rangle_{\Gamma^*} - \left(\frac{\theta^{h,n+1,i} - [D_p(\theta)]^{h,n+1,i} p(k)^{h,n+1,i} - \theta^{h,n}}{\Delta t}, \varphi\right)\\
&\quad - \left(kg^{h,n+1,i} D_x x_3, D_x\varphi\right), \quad \varphi \in \mathcal{M}^h, \quad n = 1, 2, \cdots, L-1,
\end{aligned}$$

with $p^{h,1} \in \mathcal{M}^h$ chosen to be an approximation to the initial condition $p_0(x)$.

Next, the approximation to the solution $\Phi = D_k(p)\delta k$ of (3.15)–(3.17) is defined as follows. Find $(D_k(p)\delta k)^{h,n+1} \in \mathcal{M}^h$ such that

$$\begin{aligned}
&\left([D_p(\theta)]^{h,n+\frac{1}{2}} d_t \left(D_k(p)\delta k\right)^{h,n}, \varphi\right) + \left(kg^{h,n+\frac{1}{2}} D_x \left(D_k(p)\delta k\right)^{h,n+1}, D_x\varphi\right) \qquad (6.2)\\
&\quad + \left(k[D_p(g)]^{h,n+\frac{1}{2}} D_x \left(p^{h,n+\frac{1}{2}} + x_3\right) \cdot D_x \left(D_k(p)\delta k\right)^{h,n+1}, \varphi\right)\\
&\quad = -\left(g^{h,n+\frac{1}{2}} \delta k D_x \left(p^{h,n+\frac{1}{2}} + x_3\right), D_x\varphi\right), \quad \varphi \in \mathcal{M}^h, \quad n = 1, 2, \cdots, L-1,\\
&\left(D_k(p)\delta k\right)^{h,1} = 0.
\end{aligned}$$

Finally the approximation $W(k)^{h,n}$ to the solution $W(k)$ of the adjoint problem (4.1)–(4.3) is defined as

$$W(k)^{h,n} = V(k)^{h,L-n}, \quad n = 1, \cdots, L, \qquad (6.3)$$

where $V(k)^{h,n}$ is the solution of the problem: Find $V(k)^{h,n+1} \in \mathcal{M}^h$ such that

$$\begin{aligned}
&\left([D_p(\theta)]^{h,n+\frac{1}{2}} d_t V(k)^{h,n}, \varphi\right) + \left(kg^{h,n+\frac{1}{2}} D_x V(k)^{h,n+1}, D_x\varphi\right) \qquad (6.4)\\
&\quad + \left(k[D_p(g)]^{h,n+\frac{1}{2}} D_x \left(p(k)^{h,n+\frac{1}{2}} + x_3\right) \cdot D_x V(k)^{h,n+1}, \varphi\right)\\
&\quad = \left(f^n, \varphi\right), \quad v \in \mathcal{M}^h, \quad n = 1, 2, \cdots, L-1,\\
&V(k)^{h,1} = 0.
\end{aligned}$$

The following theorem can be demonstrated using a discrete analogue of the arguments given in the proofs of Theorem 3.1 and Lemma 4.1 and applying the discrete Gronwall's lemma.

THEOREM 6.1. *Under the hypothesis of Theorem 3.1, the solutions $p(k)^{h,n}$ and $W(k)^{h,n}$ of (6.1) and (6.4) are continuous with respect to the parameter k in the following sense:*

$$\max_{1\le n\le L} \|p^{h,n}(k_1) - p^{h,n}(k_2)\|_{L^2(Q)} + \sum_n \|D_x\left(p^{h,n}(k_1) - p^{h,n}(k_2)\right)\|_{L^2(Q)}\ \Delta t \\ \le c\|k_1 - k_2\|_{L^2(Q)}, \tag{6.5}$$

$$\max_{1\le n\le L} \|W(k_1)^{h,n} - W(k_2)^{h,n}\|_{L^2(Q)} + \sum_n \|D_x\left(W(k_1)^{h,n} - W(k_2)^{h,n}\right)\|_{L^2(Q)}\ \Delta t \\ \le c\|k_1 - k_2\|_{L^2(Q)}. \tag{6.6}$$

6.1. The conjugate gradient algorithm. In order to define our conjugate gradient algorithm we need to define a discrete version of the continuous functional $\mathcal{J}(k)$ and its gradient $\mathcal{J}'_k(k)$. For this purpose we will choose a finite set $\mathcal{P}_M \subset Q$ containing the M-points where the values of the parameter k will be iteratively updated.

Since we are employing Galerkin finite element procedures, one simple choice is to use the same finite element basis associated with $\mathcal{M}^h$ to represent our parameter k, so that $\mathcal{P}_M$ is chosen to coincide with the set of nodal points $(x_m)_{1\le m\le M}$ associated with the representation of $k(x)$ in a basis of $\mathcal{M}^h$. Another possible choice is to select as $\mathcal{P}_M$ the set of all centers of the elements $Q_j \in \mathcal{T}^h$ or a subset of such centers.

Next, we define our discrete functional by

$$\mathcal{J}^h(k) = \frac{1}{2}\sum_{n=1}^{L}\sum_{i=1}^{N_r}\left(\widehat{p}^{h,n}(k,x_{ri}) - p^{obs,n}(x_{ri})\right)^2\ \Delta t. \tag{6.7}$$

Identifying k with its values $(k(x_m))_{1\le m\le M}$, $\mathcal{J}^h(k)$ can be regarded as a functional from R^M into R. Also, it follows from (6.5) and (6.7) that $\mathcal{J}^h(k)$ is a continuous linear functional with respect to the parameter k.

Next , since $(D_k(p))^{h,n} : \delta\mathcal{P}_0 \to L^2(Q)$ let us define $(\overrightarrow{D_k(p)})^h = \left((D_k(p))^{h,n}\right)_{1\le n\le L}$, so that

$$(\overrightarrow{D_k(p)})^h : \delta\mathcal{P}_0 \to [L^2(Q)]^L$$

and let $(\overrightarrow{D_k(p)})^{h,*}$ denote its adjoint:

$$(\overrightarrow{D_k(p)})^{h,*} : [L^2(Q)]^L \to \delta\mathcal{P}_0.$$

Now the following relation is a discretized form of (4.20): for any $f^{(\cdot)} \in [L^2(Q)]^L$,

$$\left((\overrightarrow{D_k(p)})^{h,*} f^{(\cdot)}, \delta k\right)_{L^2(Q)} = -\left(\sum_n g^{h,n+\frac{1}{2}} D_x\left(p^{h,n+\frac{1}{2}} + x_3\right)\cdot D_x W^{h,n+1}(k)\Delta t, \delta k\right)_{L^2(Q)}, \\ \forall \delta k \in \delta\mathcal{P}_0, \tag{6.8}$$

where $W^{h,n}(k)$ is the solution of (6.4) with right-hand side $f^{(\cdot)} = (f^n)_{1\le n\le L}$.

Next, writing

$$p(k+\delta k)^{h,n} = p(k)^{h,n} + (D_k(p)\delta k)^{h,n} + \phi(k, k+\delta k)^{h,n}, \tag{6.9}$$
$$\mathcal{J}^h(k+\delta k) = \mathcal{J}^h(k) + D_k\mathcal{J}^h(k)\delta k + R^h(k+\delta k, k),$$

the argument in Lemma 4.3 can be repeated to see that

$$\left(D_k\mathcal{J}^h(k), \delta k\right)_{L^2(Q)} = \sum_{n=1}^{L} \left((\widehat{D}_k(p)\delta k)^{h,n}, \widehat{p}(k)^{h,n} - p^{obs,n}\right)_{R^{N_r}} \Delta t, \tag{6.10}$$
$$\forall\, \delta k \in \delta\mathcal{P}_0.$$

Next, let

$$f^n(x) = \sum_{i=1}^{N_r} \frac{1}{|B_i|}\left(\widehat{p}(k, x_{ri})^{h,n} - p^{obs,n}(x_{ri})\right)\chi_{B_i}(x), \quad 1 \le n \le L, \tag{6.11}$$

and note that the right-hand side of (6.10) is

$$\sum_{n=1}^{L} \left((\widehat{D}_k(p)\delta k)^{h,n}, \widehat{p}(k)^{h,n} - p^{obs,n}\right)_{R^{N_r}} \Delta t \tag{6.12}$$
$$= \sum_{n=1}^{L}\sum_{i=1}^{N_r} \left(\frac{1}{|B_i|}\int_{B_i} (D_k(p)\delta k)^{h,n}\chi_{B_i}(x)dx\right)\left(\widehat{p}(k, x_{ri})^{h,n} - p^{obs,n}(x_{ri})\right)\Delta t$$
$$= \sum_{n=1}^{L}\int_Q (D_k(p)\delta k)^{h,n}(x) f^n(x) dx\Delta t$$
$$= \sum_{n=1}^{L}\left((D_k(p)\delta k)^{h,n}, f^n\right)_{L^2(Q)}\Delta t = \left(\overrightarrow{(D_k(p))}^{h,*} f^{(\cdot)}, \delta k\right)_{L^2(Q)}, \quad \forall \delta k \in \delta\mathcal{P}_0.$$

Thus, (6.8), (6.10) and (6.12) show that the gradient $(\mathcal{J}_k^h)'(k) = D_k\mathcal{J}^h(k)$ can be computed using the discrete analogue of (4.20):

$$(\mathcal{J}_k^h)'(k)(x) = -\sum_{n=1}^{L} g^{h,n+\frac{1}{2}}(x) D_x(p(k)^{h,n+\frac{1}{2}}(x) + x_3)\cdot D_x W(k)^{h,n+1}(x)\Delta t,$$
$$x \in Q, \tag{6.13}$$

where $W(k)^{h,n}$ is the solution of (6.4) with the right-hand side defined by (6.11).

Now Theorem 6.1 and (6.13) imply the validity of the following Lemma.

LEMMA 6.2. *Under the assumptions of Theorem 3.1, the continuous linear functional* $(\mathcal{J}_k^h)'(k) : \delta\mathcal{P}_0 \to R$ *is Lipschitz continuous with respect to the parameter* k *in the sense:*

$$\|(\mathcal{J}_k^h)'(k_1) - (\mathcal{J}_k^h)'(k_2)\|_{L^2(Q)} + \|D_x((\mathcal{J}_k^h)'(k_1) - (\mathcal{J}_k^h)'(k_2))\|_{L^2(Q)} \tag{6.14}$$
$$\le c\|k_1 - k_2\|_{L^2(Q)}.$$

Next the Polak-Ribière conjugate gradient iteration is defined as follows:

- 1) Give an initial guess $k_0(x)$, compute $p^{h,n}(k_0)$ by solving (6.1)
- 2) Compute $d_0(x_m) = -(\mathcal{J}_k^h)'(k_0)(x_m)$, $m = 1, \cdots, M$ using (6.13).
- 3) Set j=0
- 4) Compute step length α_j

$$\alpha_j = -\frac{\sum_{n=1}^{L} \left(\left(\left(D_{k_j}(p) d_j \right)^{h,n} \right)(\cdot), \left(p(k_j)^{h,n} - p^{obs,n} \right)(\cdot) \right)_{R^{N_r}}}{\sum_{n=1}^{L} \left(\left(\left(D_{k_j}(p) d_j \right)^{h,n} \right)(\cdot), \left(\left(D_{k_j}(p) d_j \right)^{h,n} \right)(\cdot) \right)_{R^{N_r}}}$$

  where $(\cdot)$ means the evaluation of the corresponding function at $x_{ri},\ i = 1, \cdots, N_r$ and $\left(D_{k_j}(p) d_j \right)^{h,n}$ is the solution of (6.2) for the choice $\delta k = d_j$.
- 5) Update $k_j(x)$ at the points x_m by the rule

$$k_{j+1}(x_m) = k_j(x_m) + \alpha_j d_j(x_m), \quad m = 1, \cdots, M$$

  and use those values to obtain the updated $k_{j+1} \in \mathcal{P}$.
- 6) Compute $p^{h,n}(k_{j+1})$ by solving (6.1)
- 7) Compute error, if convergence is achieved, stop.
- 8) Compute $(\mathcal{J}_k^h)'(k_{j+1})(x_m)$, $m = 1, \cdots, M$ using (6.13).
- 9) Compute β_{j+1} using the Polak-Ribière formula [25]

$$\beta_{j+1}^{PR} = \frac{\left((\mathcal{J}_k^h)'(k_{j+1}), (\mathcal{J}_k^h)'(k_{j+1}) - (\mathcal{J}_k^h)'(k_j) \right)_{R^M}}{\left((\mathcal{J}_k^h)'(k_j), (\mathcal{J}_k^h)'(k_j) \right)_{R^M}}$$

- 10) Compute

$$d_{j+1}(x_m) = -(\mathcal{J}_k^h)'(k_{j+1})(x_m) + \beta_{j+1}^{PR} d_j(x_m), \quad m = 1, \cdots M$$

- 11)

$$\begin{aligned} &(\mathcal{J}_k^h)'(k_j)(x_m) \leftarrow (\mathcal{J}_k^h)'(k_{j+1})(x_m), \\ &d_j(x_m) \leftarrow d_{j+1}(x_m), \quad m = 1, \cdots, M, \\ &j = j + 1, \quad \text{go to 4)} \end{aligned} \tag{6.15}$$

Note that each iteration j of the conjugate gradient algorithm described above implies the solution of one forward nonlinear problem for $p(k_j)^{h,n}$ and two linear problems to compute $(D_{k_j}(p)d_j)^{h,n}$ and $W(k_j)^{h,n}$. Also, according to the results stated above in this section, $\mathcal{J}^h(k)$ is continuously differentiable and its gradient $(\mathcal{J}_k^h)'(k)$ is Lipschitz continuous. Thus, the convergence of the the Polak-Ribière conjugate gradient iteration is insured if a line search is performed to determine the step length α_j. See for example Corollary 4.4 in [26] and Theorem 3.5 in [27] for results on the convergence of this procedure.

Since performing a line search implies the evaluation of the functional $\mathcal{J}^h(k)$ and consequently the solution of the forward problem (6.1), in our numerical experiments instead we used the value of the step length given in item 4) above, corresponding to a quadratic approximation of $\mathcal{J}(k)$. This step length performed quite well in our numerical simulations.

In the next section we present the numerical experiments showing the implementation of the Polak-Ribière conjugate gradient iteration to estimate the saturated hydraulic conductivity $k(x)$ using an hypothetical infiltration experiment in an heterogeneous soil.

7. Numerical experiments. The proposed algorithm is implemented to estimate the saturated hydraulic conductivity $k(x)$ in a vertical heterogeneous soil profile during an infiltration experiment using synthetically generated observations. The observed data p^{obs} are the pressure head values versus time at different depths obtained as the solution of the forward problem.

For the numerical test we consider a 250 cm soil profile Q consisting of four layers with the following values of saturated hydraulic conductivity

$$k(x) = \begin{cases} 4.0\ 10^{-3} \text{ cm/s} & 0 \text{ cm} \le x < 45 \text{ cm} \\ 4.5\ 10^{-3} \text{ cm/s} & 45 \text{ cm} \le x < 125 \text{ cm} \\ 6.0\ 10^{-3} \text{ cm/s} & 125 \text{ cm} \le x < 205 \text{ cm} \\ 5.5\ 10^{-3} \text{ cm/s} & 205 \text{ cm} \le x \le 250 \text{ cm}. \end{cases} \tag{7.1}$$

The other hydraulic parameters of van Genuchten model are assumed to be constant over the whole profile with $\theta_s = 0.368$, $\theta_r = 0.104$, $n = 2.0$ and $\alpha_{vg} = 0.0335$ cm^{-1}.

In the infiltration experiment, water is uniformly applied on the soil surface ($x =$ 250 cm) at a rate of 2.5 10^{-5} cm/s for a period of 10 days. The initial pressure head values are assumed to be constant and equal to -400 cm, corresponding to a relatively dry water content condition in the soil profile. The numerical test is stopped when the infiltration front reaches the bottom boundary where no-flux boundary condition is prescribed. The time step used in the numerical solution of Richard's equation (6.1), the Gâteaux derivative (6.2) and the adjoint problem (6.4) is $\Delta t = 864$ s with a uniform partition $\mathcal{T}^h$ of Q into elements Q_j of size $h = 3.33$ cm.

The pressure head values are assumed to be recorded at discrete times t_n at 16 points x_{ri} spaced 15 cm from each other. The set $\mathcal{P}_M$, where the hydraulic conductivity values are updated consists of all centers of the elements $Q_j \in \mathcal{T}^h$. Figure 1 shows simulated pressure head observations at the recording points $x = 27.5$ cm, 87.5 cm, 162.5 cm and 222.5 cm.

The initial guess for $k(x)$ in the inverse procedure is taken to be constant and equal to 5.0 10^{-3} cm/s. Figure 2 shows the initial guess and the profile updates of $k(x)$ after 10 and 50 iterations, where some oscillations in the estimated hydraulic conductivity profiles can be observed. To eliminate these oscillations and stabilize the parameter estimation procedure, a simple post-processing algorithm of the predicted hydraulic conductivity profile is implemented using weighted averages of nearest neighbors. The detailed numerical nature of weighted averaging is not important. We have observed similar numerical results when small weights are assigned to the nearest neighbors of the point where the hydraulic conductivity is estimated.

Figure 3 shows the updated hydraulic conductivity profiles of $k(x)$ after 100, 300 and 500 iterations. Numerical oscillations almost disappear after 100 iterations and the estimated profile is quite accurate except near the global boundaries where convergence is slow. Note that in this numerical example, the hydraulic conductivity values are not assumed to be known near the top surface, as it was assumed in the derivation of our parameter estimation procedure. The algorithm first quickly reaches the true hydraulic conductivity values in the interior of the domain and then slowly adjusts the true hydraulic conductivity profile near the surface and bottom boundaries.

Several choices of the observation times t_n, ranging from continuous observations to only 1 observation per day during the 10 days of the simulation time, give almost identical estimates of the hydraulic conductivity profile $k(x)$.

The behavior of the cost functional $\mathcal{J}(k)$ against the number of iterations is shown in Figure 4. This almost monotone decreasing behavior is attained by combining the

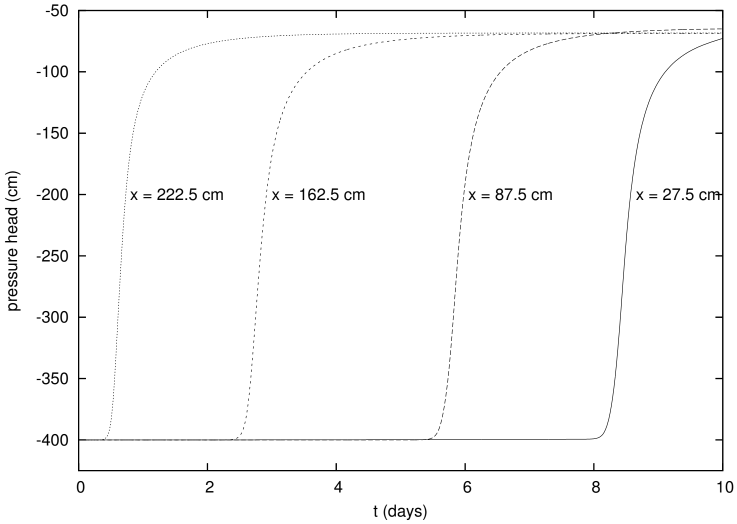

FIG. 7.1. *Simulated pressure head observations at* $x = 27.5, 87.5, 162.5$ *and* 222.5 *cm depths.*

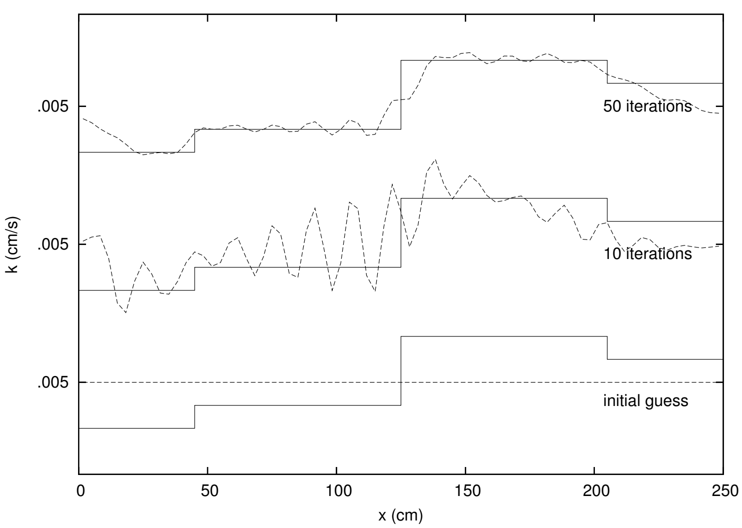

FIG. 7.2. *Initial, estimated (dashed) and true (continuous) saturated hydraulic conductivity.*

Polak-Ribière conjugate gradient iteration with a restart procedure as described in [28].

From this example, we can conclude that the proposed algorithm yields a very good estimate of saturated hydraulic conductivity in a stratified medium and becomes a promising method for *in situ* estimation of this parameter.

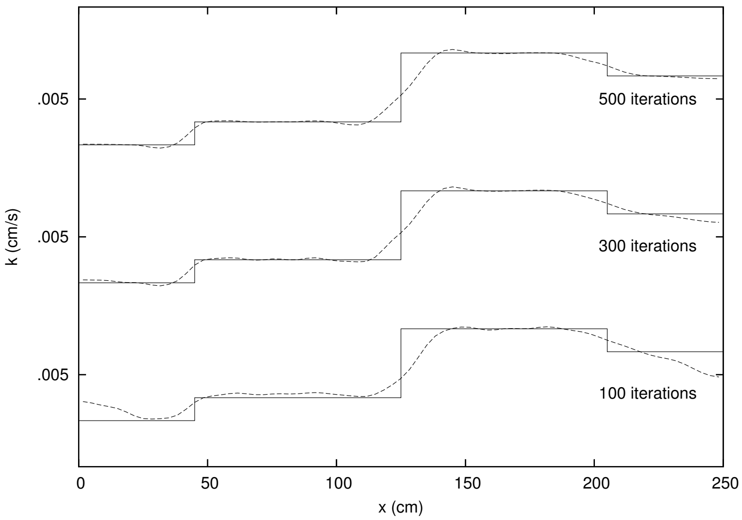

FIG. 7.3. *Estimated (dashed) and true (continuous) saturated hydraulic conductivity.*

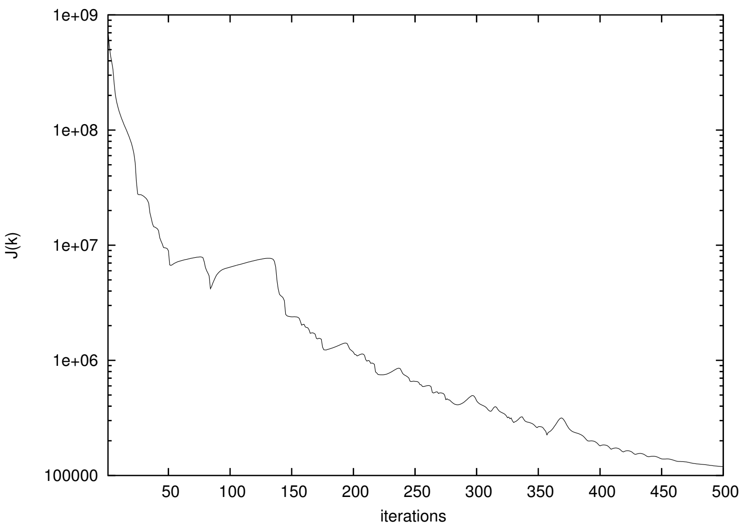

FIG. 7.4. *Cost functional.*

Appendix A. The proof of Theorem 3.1.

Proof. A weak form of equation (3.5) can be stated as follows:

$$\begin{aligned}&((D_p\theta)(p_2)D_t d_p(k_1,k_2),v) + ([(D_p\theta)(p_1) - (D_p\theta)(p_2)]\, D_t p_1, v) \\ &\quad + ((k_2 g(p_2))D_x d_p(k_1,k_2), D_x v) \\ &\quad = -\left(\zeta(k_1,k_2)D_x(p_1+x_3), D_x v\right), \quad \forall v \in H^1(Q).\end{aligned} \tag{A.1}$$

Take $v = d_p(k_1, k_2)$ in (A.1) to obtain the equation

$$\frac{1}{2}D_t\left((D_p\theta)(p_2)d_p(k_1,k_2),d_p(k_1,k_2)\right)+\left(k_2 g(p_2)D_x d_p(k_1,k_2),D_x d_p(k_1,k_2)\right)$$
$$\begin{aligned}
&=\frac{1}{2}\Big((D_p^{(2)}\theta)(p_2)(D_t p_2)d_p(k_1,k_2),d_p(k_1,k_2)\Big)\\
&-\left(\left[(D_p\theta)(p_1)-(D_p\theta)(p_2)\right]D_t p_1,d_p(k_1,k_2)\right)\\
&-\left(\zeta(k_1,k_2)D_x(p_1+x_3),D_x d_p(k_1,k_2)\right)\\
&=T_1+T_2+T_3.
\end{aligned}\tag{A.2}$$

Now we bound T_1, T_2 and T_3. First, using that $(D_p^{(2)}\theta)(p)$ and $D_t p(k)$ are bounded and that $(D_p\theta)(p)$ is Lipschitz continuous,

$$|T_1|+|T_2|\le c\|d_p(k_1,k_2)\|^2_{L^2(Q)}.\tag{A.3}$$

Next, using that $g(p)$ is bounded and Lipschitz continuous and $D_x p(k)$ is bounded

$$|T_3|\le\epsilon\|D_x d_p(k_1,k_2)\|^2_{L^2(Q)}+c\Big(\|d_p(k_1,k_2)\|^2_{L^2(Q)}+\|k_1-k_2\|^2_{L^2(Q)}\Big),\tag{A.4}$$

where $\epsilon>0$ is an arbitrary (small) constant. Using the estimates in (A.3),(A.4) in (A.2) and that (2.4) we get the inequality

$$\begin{aligned}
&\frac{1}{2}D_t\left((D_p\theta)(p_2)d_p(k_1,k_2),d_p(k_1,k_2)\right)+(c_1-\epsilon)\|D_x d_p(k_1,k_2))\|^2_{L^2(Q)}\\
&\quad\le c\Big(\|d_p(k_1,k_2)\|^2_{L^2(Q)}+\|k_1-k_2\|^2_{L^2(Q)}\Big).
\end{aligned}\tag{A.5}$$

Since $d_p(k_1,k_2)(t=0)=0$, choosing ϵ sufficiently small, we integrate (A.5) with respect to time and use (2.5) to get the estimate

$$\begin{aligned}
&\|d_p(k_1,k_2)\|^2_{L^2(Q)}(t)+\int_0^t\|D_x d_p(k_1,k_2)\|^2_{L^2(Q)}(\tau)d\tau\\
&\quad\le c\int_0^t\Big(\|d_p(k_1,k_2)\|^2_{L^2(Q)}(\tau)+\|k_1-k_2\|^2_{L^2(Q)}\Big)d\tau.
\end{aligned}\tag{A.6}$$

Using Gronwall's lemma in (A.6) we obtain (3.10) for $n=0$.

Next we proceed to obtain the estimate (3.10) for $n=1$, i.e., for $Z(k_1,k_2)=D_t d_p(k_1,k_2)$. Recall that for any function $f(p(k))$, we denote

$$d_f(k_1,k_2)=f(p_1)-f(p_2).$$

Then taking time derivatives in (3.5),(3.6), (3.7) and (3.8), we obtain that $Z(k_1,k_2)$ satisfies the equations

$$\begin{aligned}
&(D_p^{(2)}\theta)(p_2)(D_t p_2)Z(k_1,k_2)+(D_p\theta)(p_2)D_t Z(k_1,k_2)\\
&\quad+D_t(d_{D_p\theta}(k_1,k_2))D_t p_1+d_{D_p\theta}(k_1,k_2)D_t^{(2)}p_1\\
&\quad-div\left(k_2(D_p g)(p_2)(D_t p_2)D_x d_p(k_1,k_2)\right)\\
&\quad-div\left(k_2 g(p_2)D_x Z(k_1,k_2)\right)\\
&\quad=div\left((D_t\zeta(k_1,k_2))D_x(p_1+x_3)\right)+div\left(\zeta(k_1,k_2)D_x D_t p_1\right),\quad x\in Q,t\in I,
\end{aligned}\tag{A.7}$$

with the boundary conditions

$$
\begin{aligned}
&-k_2 g(p_2) D_x Z(k_1,k_2)\cdot\nu - k_2 (D_p g)(p_2)(D_t p_2) D_x d_p(k_1,k_2)\cdot\nu \\
&\quad = (D_t\zeta(k_1,k_2)) D_x(p_1+x_3)\cdot\nu + \zeta(k_1,k_2) D_x D_t p_1\cdot\nu, \quad x\in\Gamma^*, t\in I, \\
&-k_2 g(p_2) D_x Z(k_1,k_2)\cdot\nu = 0, \quad x\in\Gamma, t\in I,
\end{aligned} \tag{A.8}
$$

and initial condition

$$
Z(k_1,k_2)(\cdot,t=0)=0, \quad x\in Q. \tag{A.9}
$$

A weak form for (A.7)-(A.8) is as follows:

$$
\begin{aligned}
&\left((D_p^{(2)}\theta)(p_2)(D_t p_2) Z(k_1,k_2), v\right) + ((D_p\theta)(p_2) D_t Z(k_1,k_2), v) + (k_2 g(p_2) D_x Z(k_1,k_2), D_x v) \\
&\quad = -\left(D_t(d_{D_p\theta}(k_1,k_2)) D_t p_1, v\right) - \left(d_{D_p\theta}(k_1,k_2) D_t^{(2)} p_1, v\right) \\
&\qquad - (k_2 (D_p g)(p_2)(D_t p_2) D_x d_p(k_1,k_2), D_x v) - ((D_t\zeta(k_1,k_2)) D_x(p_1+x_3), D_x v) \\
&\qquad - (\zeta(k_1,k_2) D_x D_t p_1, D_x v), \qquad \forall v\in H^1(Q).
\end{aligned} \tag{A.10}
$$

Taking $v = Z(k_1,k_2)$ in (A.10), we obtain the equation

$$
\begin{aligned}
&\frac{1}{2} D_t\left((D_p\theta)(p_2) Z(k_1,k_2), Z(k_1,k_2)\right) + (k_2 g(p_2) D_x Z(k_1,k_2), D_x Z(k_1,k_2)) \\
&\quad = -\frac{1}{2}\left((D_p^{(2)}\theta)(p_2) D_t(p_2) Z(k_1,k_2), Z(k_1,k_2)\right) \\
&\quad - \left(D_t(d_{D_p\theta}(k_1,k_2)) D_t p_1, Z(k_1,k_2)\right) - \left(d_{D_p\theta}(k_1,k_2) D_t^{(2)} p_1, Z(k_1,k_2)\right) \\
&\quad - (k_2 (D_p g)(p_2)(D_t p_2) D_x d_p(k_1,k_2), D_x Z(k_1,k_2)) \\
&\quad - (\zeta(k_1,k_2) D_x D_t p_1, D_x Z(k_1,k_2)) \\
&\quad - ((D_t\zeta(k_1,k_2)) D_x(p_1+x_3), D_x Z(k_1,k_2)) \\
&\quad = T_4+T_5+T_6+T_7+T_8+T_9.
\end{aligned} \tag{A.11}
$$

Next we bound T_i, $i=4,5,6,7,8,9$. First, we note that

$$
D_t(d_{(D_p\theta)}(k_1,k_2)) = (D_p^{(2)}\theta)(p_1) Z(k_1,k_2) + d_{(D_p^{(2)}\theta)}(k_1,k_2) D_t p_2, \tag{A.12}
$$

and

$$
\begin{aligned}
D_t\zeta(k_1,k_2) = {}& k_1\left[(D_p g)(p_1) Z(k_1,k_2) + d_{D_p g}(k_1,k_2) D_t p_2\right] \\
&+ (D_p g)(p_2) D_t p_2 \left[k_1 - k_2\right].
\end{aligned} \tag{A.13}
$$

Then, using (A.12), and the facts that that $(D_p^{(2)}\theta)(p), D_t p(k)$, and $D_t^{(2)} p(k)$ are bounded and that $(D_p\theta)(p)$, $(D_p^{(2)}\theta)(p)$ are Lipschitz continuous functions, we obtain that

$$
|T_4| + |T_5| + |T_6| \le c\left(\|Z(k_1,k_2)\|^2_{L^2(Q)} + \|d_p(k_1,k_2)\|^2_{L^2(Q)}\right). \tag{A.14}
$$

Next, using the facts that that $g(p)$ is bounded and Lipschitz continuous and that $D_t p, (D_p g)(p)$ are bounded, we get

$$
\begin{aligned}
|T_7| + |T_8| \le {}& \epsilon\|D_x Z(k_1,k_2)\|^2_{L^2(Q)} + c\Big(\|Z(k_1,k_2)\|^2_{L^2(Q)} \\
&+ \|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|k_1 - k_2\|^2_{L^2(Q)}\Big).
\end{aligned} \tag{A.15}
$$

Finally, using (A.13), that $(D_p g)(p)$ is bounded and Lipschitz continuous and that $D_x p, D_t p$ are bounded,

$$|T_9| \leq \epsilon \|D_x Z(k_1,k_2)\|^2_{L^2(Q)} + c\left(\|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|Z(k_1,k_2)\|^2_{L^2(Q)} \right. \tag{A.16}$$
$$\left. +\|k_1 - k_2\|^2_{L^2(Q)}\right).$$

Using the bounds for $T_i,\ i = 4, \cdots, 9$ and (2.4) in (A.11), for ϵ appropriately chosen we get the inequality

$$\frac{1}{2} D_t\left((D_p\theta)(p_2)Z(k_1,k_2), Z(k_1,k_2)) + \|D_x Z(k_1,k_2))\|^2_{L^2(Q)}\right.$$
$$\leq c\left(\|Z(k_1,k_2)\|^2_{L^2(Q)} + \|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|k_1 - k_2\|^2_{L^2(Q)}\right). \tag{A.17}$$

Integrate (A.17) with respect to time, using (2.5) and applying Gronwall's lemma in the resulting equation, we obtain (3.10) for $n = 1$.

Finally, we proceed to derive the estimate (3.10) for $n = 2$. First, we take the time derivative of (A.7)-((A.9) and set

$$U(k_1,k_2) = D_t Z(k_1,k_2)$$

and obtain

$$\begin{aligned}
&(D_p^{(3)}\theta)(p_2)(D_t p_2)^2 Z(k_1,k_2) + (D_p^{(2)}\theta)(p_2)(D_t^{(2)} p_2)Z(k_1,k_2) \\
&\quad +2(D_p^{(2)}\theta)(p_2)(D_t p_2)U(k_1,k_2) \\
&\quad +(D_p\theta)(p_2)D_t U(k_1,k_2) + D_t^{(2)}(d_{D_p\theta}(k_1,k_2))D_t p_1 \\
&\quad +2D_t(d_{D_p\theta}(k_1,k_2))D_t^{(2)} p_1 + d_{Dp\theta}(k_1,k_2)D_t^{(3)} p_1 \\
&\quad -div\left(k_2(D_p^{(2)} g)(p_2)(D_t p_2)^2 D_x d_p(k_1,k_2)\right) - 2div\left(k_2(D_p g)(p_2)(D_t p_2)D_x Z(k_1,k_2)\right) \\
&\quad -div\left(k_2 g(p_2)D_x U(k_1,k_2)\right) \\
&\quad = div\left((D_t^{(2)}\zeta(k_1,k_2))D_x(p_1 + x_3)\right) + 2div\left((D_t\zeta(k_1,k_2))D_x D_t p_1\right) \\
&\qquad +div\left(\zeta(k_1,k_2)D_x D_t^{(2)} p_1\right), \quad x \in Q, t \in I,
\end{aligned} \tag{A.18}$$

with the boundary condition

$$\begin{aligned}
&-k_2 g(p_2)D_x U(k_1,k_2)\cdot\nu - 2k_2(D_p g)(p_2)(D_t p_2)D_x Z(k_1,k_2)\cdot\nu \\
&\quad -k_2(D_p^{(2)} g)(p_2)(D_t p_2)^2 D_x d_p(k_1,k_2)\cdot\nu \\
&\quad = (D_t^{(2)}\zeta(k_1,k_2))D_x(p_1 + x_3)\cdot\nu + 2(D_t\zeta(k_1,k_2))D_x D_t p_1\cdot\nu \\
&\qquad +\zeta(k_1,k_2)D_x D_t^{(2)} p_1\cdot\nu, \quad x \in \Gamma^*, t \in I, \\
&-k_2 g(p_2)D_x U(k_1,k_2)\cdot\nu = 0, \quad x \in \Gamma, t \in I,
\end{aligned} \tag{A.19}$$

and the initial condition

$$U(k_1,k_2)(\cdot, t = 0) = 0, \quad x \in Q. \tag{A.20}$$

A weak form for (A.18)-(A.19) is as follows:

$$
\begin{aligned}
&\left((D_p^{(3)}\theta)(p_2)(D_tp_2)^2Z(k_1,k_2),v\right)+\left((D_p^{(2)}\theta)(p_2)(D_t^{(2)}p_2)Z(k_1,k_2),v\right) \qquad \text{(A.21)}\\
&\quad +2\left((D_p^{(2)}\theta)(p_2)(D_tp_2)U(k_1,k_2),v\right)\\
&\quad +((D_p\theta)(p_2)D_tU(k_1,k_2),v)+\left(D_t^{(2)}(d_{D_p\theta}(k_1,k_2))D_tp_1,v\right)\\
&\quad +2\left(D_t(d_{D_p\theta}(k_1,k_2))D_t^{(2)}p_1,v\right)+\left(d_{Dp\theta}(k_1,k_2)D_t^{(3)}p_1,v\right)\\
&\quad +\left(k_2(D_p^{(2)}g)(p_2)(D_tp_2)^2D_xd_p(k_1,k_2),D_xv\right)+2\left(k_2(D_pg)(p_2)(D_tp_2)D_xZ(k_1,k_2),D_xv\right)\\
&\quad +(k_2g(p_2)D_xU(k_1,k_2),D_xv)\\
&\quad =-\left((D_t^{(2)}\zeta(k_1,k_2))D_x(p_1+x_3),D_xv\right)-2\left((D_t\zeta(k_1,k_2))D_xD_tp_1,D_xv\right)\\
&\qquad -\left(\zeta(k_1,k_2)D_xD_t^{(2)}p_1,D_xv\right),\quad x\in Q,t\in I.
\end{aligned}
$$

Now take $v=U(k_1,k_2)$ in (A.21) to obtain the equation

$$
\begin{aligned}
&\frac{1}{2}D_t\left((D_p\theta)(p_2)U(k_1,k_2),U(k_1,k_2)\right)+(k_2g(p_2)D_xU(k_1,k_2),D_xU(k_1,k_2)) \qquad \text{(A.22)}\\
&\quad =-\frac{3}{2}\left((D_p^{(2)}\theta)(p_2)(D_tp_2)U(k_1,k_2),U(k_1,k_2)\right)-\left((D_p^{(3)}\theta)(p_2)(D_tp_2)^2Z(k_1,k_2),U(k_1,k_2)\right)\\
&\quad -\left((D_p^{(2)}\theta)(p_2)(D_t^{(2)}p_2)Z(k_1,k_2),U(k_1,k_2)\right)\\
&\quad -\left(D_t^{(2)}(d_{D_p\theta}(k_1,k_2))D_tp_1,U(k_1,k_2)\right)-2\left(D_t(d_{D_p\theta}(k_1,k_2))D_t^{(2)}p_1,U(k_1,k_2)\right)\\
&\quad -\left(d_{Dp\theta}(k_1,k_2)D_t^{(3)}p_1,U(k_1,k_2)\right)-\left(k_2(D_p^{(2)}g)(p_2)(D_tp_2)^2D_xd_p(k_1,k_2),D_xU(k_1,k_2)\right)\\
&\quad -2\left(k_2(D_pg)(p_2)(D_tp_2)D_xZ(k_1,k_2),D_xU(k_1,k_2)\right)\\
&\quad -\left((D_t^{(2)}\zeta(k_1,k_2))D_x(p_1+x_3),D_xU(k_1,k_2)\right)\\
&\quad -2\left((D_t\zeta(k_1,k_2))D_xD_tp_1,D_xU(k_1,k_2)\right)-\left(\zeta(k_1,k_2)D_xD_t^{(2)}p_1,D_xU(k_1,k_2)\right)\\
&= \qquad \sum_{i=10}^{i=20}T_i. \qquad \text{(A.23)}
\end{aligned}
$$

Next, we bound each T_i on the right-hand side of (A.22). First, using the facts that $(D_p^{(2)}\theta)(p),(D_p^{(3)}\theta)(p),D_tp(k)$ and $D_t^{(2)}p(k)$ are bounded, we obtain

$$
|T_{10}|+|T_{11}|+|T_{12}|\le c\left(\|Z(k_1,k_2)\|^2_{L^2(Q)}+\|U(k_1,k_2)\|^2_{L^2(Q)}\right). \qquad \text{(A.24)}
$$

Next, from (A.12) we get

$$
\begin{aligned}
D_t^{(2)}(d_{D_p\theta}(k_1,k_2)) &= (D_p^{(3)}\theta)(p_1)(D_tp_1)Z(k_1,k_2)+d_{D_p^{(2)}\theta}(k_1,k_2)D_t^{(2)}p_2\\
&\quad +\left[(D_p^{(3)}\theta)(p_1)Z(k_1,k_2)+d_{D_p^{(3)}\theta}(k_1,k_2)D_tp_2\right]D_tp_2\\
&\quad +(D_p^{(2)}\theta)(p_1)H(k_1,k_2).
\end{aligned}
$$

Thus, using that $(D_p\theta)(p),(D_p^{(2)}\theta)(p),(D_p^{(3)}\theta)(p)$ are bounded and Lipschitz continuous functions and $D_t p(k), D_t^{(2)} p(k), D_t^{(3)} p(k)$ are bounded, we get

$$|T_{13}| + |T_{14}| + |T_{15}| \le c\left(\|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|Z(k_1,k_2)\|^2_{L^2(Q)} + \|U(k_1,k_2)\|^2_{L^2(Q)} \right). \tag{A.25}$$

Moreover, since $(D_p g)(p), (D_p^{(2)} g)(p), D_t p$ are bounded, we have

$$|T_{16}| + |T_{17}| \le \epsilon \|D_x U(k_1,k_2)\|^2_{L^2(Q)} + c\left(\|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|Z(k_1,k_2)\|^2_{L^2(Q)} \right). \tag{A.26}$$

Next, using (A.13), we obtain that

$$\begin{aligned} D_t^{(2)} \zeta(k_1,k_2) = {} & k_1 \left[(D_p^{(2)} g)(p_1)(D_t p_1) Z(k_1,k_2) + (D_p g)(p_1) U(k_1,k_2) \right] \\ & + \left[(D_p^{(2)} g)(p_1) Z(k_1,k_2) + d_{D_p^{(2)} g}(k_1,k_2) \right] D_t p_2 \\ & + d_{D_p g}(k_1,k_2) D_t^{(2)} p_2 + \left[(D_p^{(2)} g)(p_2)(D_t p_2)^2 + (D_p g)(p_2) D_t^{(2)} p_2 \right] [k_1 - k_2]. \end{aligned} \tag{A.27}$$

Thus, using (A.13), (A.27) and the facts that $g(p), (D_p g)(p), (D_p^{(2)} g)(p)$ are bounded and Lipschitz continuous functions and $D_t p(k), D_t^{(2)} p(k), D_x p(k)$ are bounded, we get

$$\begin{aligned} |T_{18}| + |T_{19}| + |T_{20}| \le {} & \epsilon \|D_x U(k_1,k_2)\|^2_{L^2(Q)} + c\Big(\|d_p(k_1,k_2)\|^2_{L^2(Q)} \\ & + \|Z(k_1,k_2)\|^2_{L^2(Q)} + \|U(k_1,k_2)\|^2_{L^2(Q)} + \|k_1 - k_2\|^2_{L^2(Q)} \Big). \end{aligned} \tag{A.28}$$

Collecting the bounds for $T_i,\ i = 10, 20$ and choosing ϵ appropriately, from (A.22) we obtain

$$\begin{aligned} & \frac{1}{2} D_t \left((D_p \theta)(p_2) U(k_1,k_2), U(k_1,k_2) \right) + \|D_x U(k_1,k_2))\|^2_{L^2(Q)} \\ & \le c\Big(\|U(k_1,k_2)\|^2_{L^2(Q)} + \|Z(k_1,k_2)\|^2_{L^2(Q)} + \|D_x Z(k_1,k_2)\|^2_{L^2(Q)} \\ & + \|d_p(k_1,k_2)\|^2_{L^2(Q)} + \|D_x d_p(k_1,k_2)\|^2_{L^2(Q)}\| + \|k_1 - k_2\|^2_{L^2(Q)} \Big). \end{aligned} \tag{A.29}$$

Integrating (A.29) with respect to time, using (2.5) and (2.4), and applying Gronwall's lemma in the resulting equation and using the estimates (3.10) already derived for $n = 0, 1$ we obtain

$$\begin{aligned} & \|D_t^{(2)} d_p(k_1,k_2)\|_{L^\infty(I,L^2(Q)} + \|D_x D_t^{(2)} d_p(k_1,k_2)\|_{L^2(I,L^2(Q))} \\ & \le c\big(\|d_p(k_1,k_2)\|_{L^2(I,L^2(Q))} + \|D_x d_p(k_1,k_2)\|_{L^2(I,L^2(Q)} \\ & + \|D_t d_p(k_1,k_2)\|_{L^2(I,L^2(Q))} + \|D_x D_t d_p(k_1,k_2)\|_{L^2(I,L^2(Q))} \\ & + \|k_1 - k_2\|_{L^2(I,L^2(Q)))} \big) \\ & \le c\|k_1 - k_2\|_{L^2(I,L^2(Q))}. \end{aligned} \tag{A.30}$$

This completes the proof. ☐

REFERENCES

[1] R. H. Brooks and A. T. Corey, Hydraulic properties of porous media, Hydrology Paper 3, Colorado State University, Fort Collins, 1964.
[2] M. T. van Genutchen, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils: Soil Sci. Soc. Am. J., v. 44 (1980) 892-898.
[3] J. H. Dane and S. Hurska, In situ determination of soil hydraulic properties during drainage: Soil Sci. Soc. Am. J. 58 (1983) 647-652.
[4] Z. Y. Zou, M. H. Young, Z. Li and P. J. Wierenga, Estimation of depth average unsaturated soil hydraulic properties from infiltration experiments: Journal of Hydrology 242 (2001) 26-42.
[5] J. Simunek and M. T. van Genutchen, Estimating unsaturated soil hydraulic properties from tension disc infiltrometer data by numerical inversion, Water. Resour. Res. 32 (1996) 2683-2696.
[6] G. A. Olyphant, Temporal and spatial (down profile) variability of unsaturated soil hydraulic properties determined from a combination of repeated field experiments and inverse modeling, Journal of Hydrology 281 (2003), 23-35.
[7] J. Zijlstra and J. H. Dane, Identification of hydraulic parameters in layered soils based on a quasi-Newton method: Journal of Hydrology 181 (1996) 233-250.
[8] G. N utzmann, M. Thiele, S. Maciejewski and K. Joswig, Inverse modelling techniques for determining hydraulic properties of coarse-textured porous media by transient outflow methods, Adv. in Water Res. 22 (1998) 273-284.
[9] K. C. Abbaspour, R. Schulin, M. T. van Genuchten, Estimating unsaturated soil hydraulic parameters using ant colony optimization, Adv. in Water Res. 24 (2001) 827-841.
[10] J. H. Dane and J. F. Molz, Physical measurements in subsurface hydrology, Rev. Geophys., Suppl. (1991) 270-279.
[11] J. B. Kool, J. C. Parker and M. T. van Genuchten, Parameter estimation for unsaturated flow and transport models–a review: Journal of Hydrology 91 (1987) 255-293.
[12] L. Richards, Capillary conduction of liquids through porous mediums: Physics, v. 1 (1931) 318-333.
[13] A. Tarantola, A., Linearized inversion of seismic reflection data, Geophysical Prospecting, 32 (1984) 998–1015.
[14] A. Tarantola, A., Inverse Problem Theory, Elsevier, New York, 1987.
[15] Y. Jarny, M. N. Ozisik and J. P. Bardon, A general optimization method using the adjoint equation for solving multidimensional inverse heat conduction, Int. J. Heat and Mass Transfer, 47 (1986) 2911-2919.
[16] E. M. Fenandez-Berdaguer, Parameter estimation in acoustic media using the adjoint method, SIAM J. Control Optim., 36 (1998) 1315–1330.
[17] R. Sampath and N. Zabara, A functional optimization approach to an inverse magneto-convection problem, Comput. Methods in Appl. Mech. Engrg. 190 (2002) 2063–2097.
[18] E. M. Fenandez-Berdaguer, L. V. Perez and J. E. Santos, Numerical experiments on parameter estimation in acoustic media using the adjoint method, Latin American Applied Research, 32 (2002) 337–342.
[19] H. T. Banks and K. Kunish, Estimation techniques for distributed parameter systems, Birkhauser, Boston, 1989.
[20] L. Lines and S. Treitel, A review of least-squares inversion and its application to geophysical problems, Geophysical Prospecting, 32 (1984) 159–186.
[21] M. G. Armentano, E. M. Fernández-Berdaguer and J. E. Santos, J. E., A frequency domain parameter estimation procedure in viscoelastic layered media, Computational and Applied Mathematics, 14 (1995) 191–216.
[22] E. M. Fernández Berdaguer, J. E. Santos and D. Sheen, An iterative procedure for estimation of variable coefficients in a hyperbolic system, Applied Mathematics and Computation, 76 (1996) 210–250.
[23] E. M. Fernández Berdaguer and J. E. Santos, On the solution of an inverse scattering problem in one-dimensional acoustic media, Comput. Methods Appl. Mech. Engrg. 129 (1996) 91–105.
[24] J. E. Santos, On the solution of an inverse scattering problem in seismic while-drilling technology, Comp. Methods Appl. Mech. and Engrg. 191 (2002) 2403–2425.
[25] E. Polak et G. Ribière, Note sur la convergence de méthodes de directions conjuguées, Revue Fr. Inf. Rech. Oper., 16-R1 (1969) 35-43.
[26] J. C. Gilbert and J. Nocedal, Global convergence of conjugate gradient methods for optimization, SIAM J. Optimization, 2 (1) (2002), 21-42.
[27] Y. Dai, J. Han, G. Liu, D. Sun, H. Yin and Y. Yuan, Convergence properties of nonlinear conjugate gradient methods, SIAM J. Optimization, 10 (2) (1999) 345–358.
[28] M. J. D. Powell, Restart procedures for the conjugate gradient method, mathematical Programming, 12 (1977) 241–254.